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# Open-source bandstructure models of interdiffusion, impurity and exciton states for the Quantum Wells, Wires and Dots (QWWAD) simulation suite

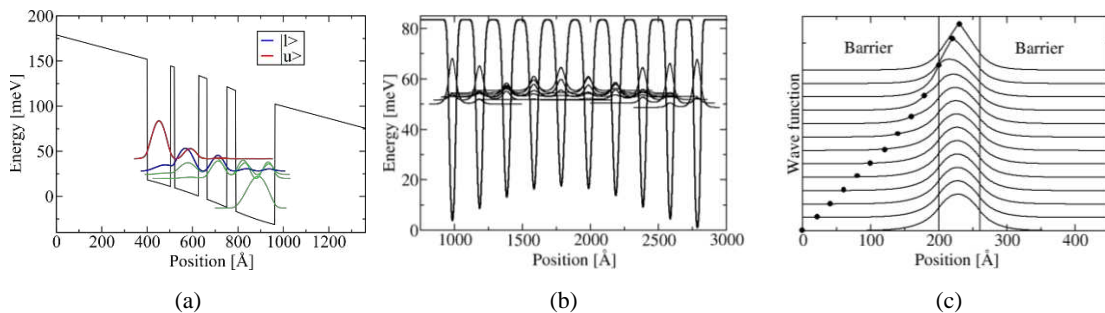
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The vast majority of high-quality software for simulating semiconductor nanostructures (e.g., [1]) is supplied under a proprietary license and its source code cannot be studied, modified or redistributed by its users. The open-source project, Quantum Wells, Wires and Dots (QWWAD) [2] is a free, non-commercial community-focused resource, which accompanies the new 4<sup>th</sup> edition of the eponymous textbook [3]. Previously described features in QWWAD include numerical Schrodinger/Poisson solvers in generic 1D potentials [e.g., Fig. 1(a)], quasi-analytical and empirical pseudopotential calculations of the band-structure in quantum wires and dots, and scattering calculations for interactions with impurities, phonons, interface roughness, alloy disorder and carrier-carrier processes. We describe new tools, included in the latest release (QWWAD v1.4), for modelling the perturbed quantum-confined states within 2D heterostructures resulting from interdiffusion, impurities and excitonic contributions.



**Fig. 1:** (a) Self-consistent Poisson–Schrödinger solution for a THz QCL using tight-binding boundary conditions. (b) Potential profile (bold) and electron probability densities (feint) in a multi-quantum-well system after simulated annealing, using a constant diffusion coefficient. (c) Wave functions for 1s state of an electron interacting with a donor at a range of locations (indicated by circles) within a quantum well, assuming a spherically symmetrical hydrogenic factor.

In QWWAD v1.4, diffuse bandstructure is simulated using numerical solutions to a Fick annealing model, with the diffusion coefficient being either constant or a function of diffusant concentration, time or position within the heterostructure [Fig. 1(b)]. Quasi-analytical models of 1s-states for impurities in heterostructures (with cylindrically, spherically or ellipsoidally symmetric orbitals) [Fig. 1(c)]. Numerical variational solvers enable the calculation of higher-order s- and p-states. Excitonic states are also computed using a similar set of models.

Development of QWWAD is coordinated through a community-focused project on the Launchpad website [3]. A hierarchical software architecture allows considerable flexibility in its usage, including a C++ Application Programmers Interface, “building-block” programs for common modelling tasks and a set of example UNIX scripts suitable for non-expert users.

[1] Nextnano, <http://www.nextnano.de>

[2] Quantum wells, wires and dots (QWWAD), <http://launchpad.net/qwwad>

[3] P. Harrison and A. Valavanis, Quantum Wells, Wires and Dots, 4<sup>th</sup> Ed. Wiley, Chichester (2016).